

SUPPLEMENTAY MATERIAL

Precise Measurement of RDCs in Water and DMSO based Gels Using a Silicone Rubber Tube for Variable Stretching

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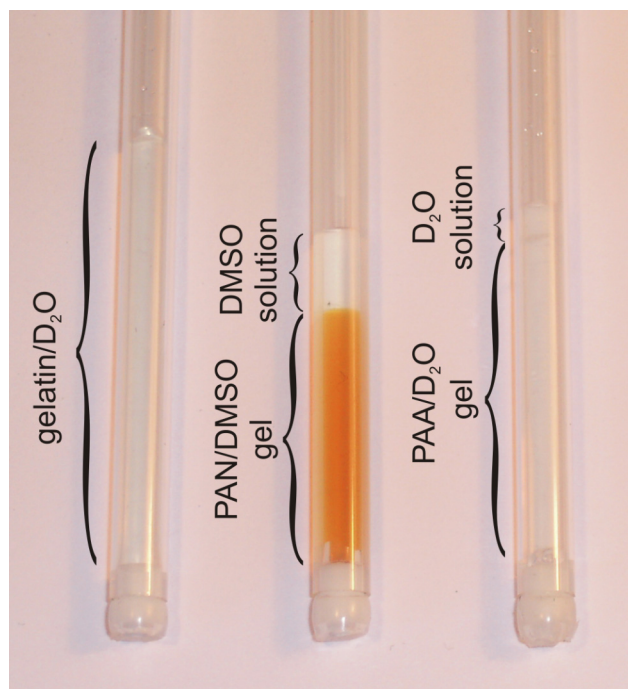
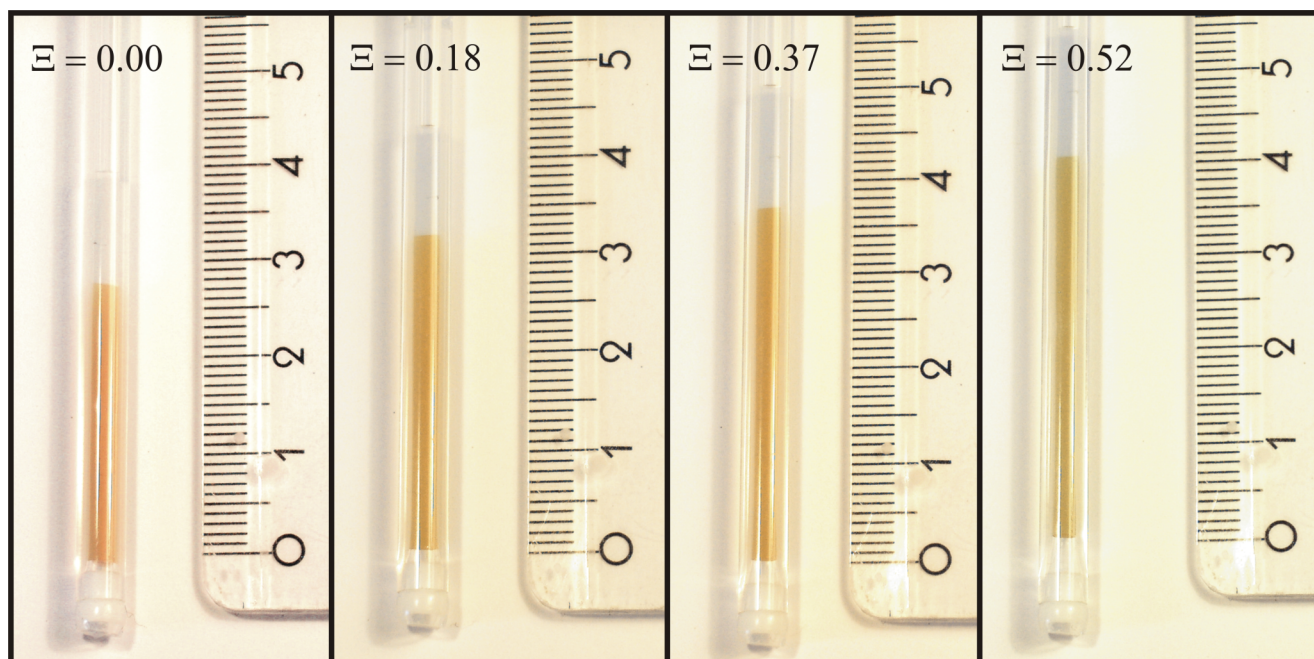
Fig. (S1). Various gels used to extract RDCs with the stretching apparatus. From left to right: gelatin/D₂O, PAN/DMSO and PAA/D₂O.

Fig. (S2). Stretching apparatus with a PAN/DMSO gel at various extensions.

Linear regressions of $^1T_{CH}$ couplings with respect to the quadrupolar splittings $\Delta\nu_Q$ as shown in Fig. (3) were done with the Linear Fit option of OriginPro 7.5G. Fit parameters A and B of the regression equation $Y = A + B \cdot X$, with Y being measured $^1T_{CH}$ couplings and X being the corresponding $\Delta\nu_Q$ values, are given in Tables S1-S3 for all CH-couplings of sucrose in the different alignment media used. Furthermore, maximum deviations of the measured $^1T_{CH}$ couplings from the linear fit ($\max. \Delta^1T_{CH}$) and root mean square deviations ($\sigma (^1T_{CH})$) of all the measured couplings are given.

Table S1. Fit Parameters for $^1T_{CH}$ Couplings of Sucrose Measured in Gelatin/D₂O

Signal	A [Hz]	B	max. Δ^1T_{CH} [Hz]	$\sigma (^1T_{CH})$ [Hz]
1'	169.17± 0.18	0.147± 0.001	1.6 /-1.0	0.53
2'	145.33± 0.19	0.042± 0.001	1.1 /-1.0	0.63
3'	145.03± 0.36	0.043± 0.002	1.7 /-2.6	1.13
4'	145.86± 0.49	0.022± 0.003	1.9 /-2.6	1.54
5'	145.60± 0.38	0.050± 0.002	2.1 /-1.9	1.16
3	144.92± 0.15	-0.059± 0.001	0.6 /-1.1	0.49
4	146.76± 0.31	-0.010± 0.002	2.3 /-1.9	1.14
5	148.87± 0.36	-0.189± 0.002	2.1 /-2.0	1.11

Table S2. Fit Parameters for $^1T_{CH}$ Couplings of Sucrose Measured in PAA/D₂O

Signal	A [Hz]	B	max. Δ^1T_{CH} [Hz]	$\sigma (^1T_{CH})$ [Hz]
1'	144.15± 0.02	0.115± 0.010	0.1 /-0.5	0.3
3'	145.42± 0.43	0.217± 0.014	0.6 /-0.6	0.4
4'	143.23± 0.79	0.180± 0.027	0.3 /-1.3	0.6
5'	147.53± 0.33	-0.318± 0.014	0.3 /-0.4	0.6
3	145.84± 0.25	-0.333± 0.010	0.6 /-0.4	0.4
4	149.81± 0.40	-0.443± 0.015	0.6 /-1.6	0.8
5	169.97± 0.13	0.220± 0.005	0.2 /-0.1	0.1

Table S3. Fit Parameters for $^1T_{CH}$ Couplings of Sucrose Measured in PAN/DMSO

Signal	A [Hz]	B	max. Δ^1T_{CH} [Hz]	$\sigma (^1T_{CH})$ [Hz]
1'	167.42± 0.10	0.372± 0.006	0.4 /-0.5	0.26
2'	141.00± 0.10	0.182± 0.006	0.5 /-0.4	0.25
3'	143.12± 0.23	0.184± 0.014	0.9 /-0.8	0.59
4'	141.76± 0.18	0.089± 0.011	1.0 /-0.8	0.46
5'	143.22± 0.34	0.168± 0.022	2.4 /-2.0	0.89
3	141.47± 0.22	-0.392± 0.014	0.9 /-1.2	0.57
4	141.54± 0.27	-0.320± 0.018	1.3 /-1.1	0.72
5	145.99± 0.19	-0.426± 0.012	1.2 /-0.8	0.50

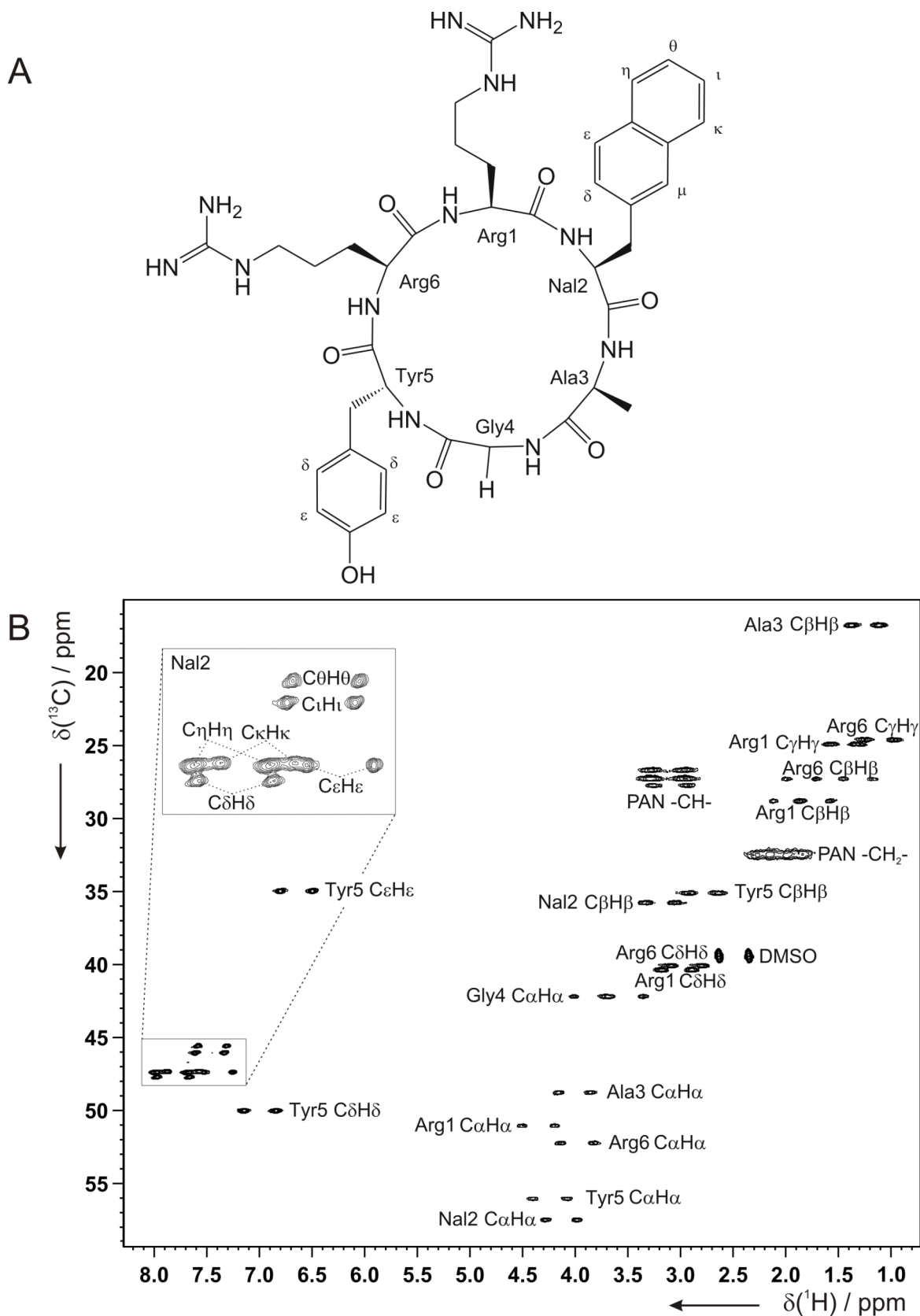


Fig. (S3). Structure (A) and CLIP-HSQC spectrum (B) of the cyclic hexapeptide cyclo(Arg-Nal-Ala-Gly-D-Tyr-Arg) in the unstretched PAN/DMSO gel.